



Next Generation Cyberinfrastructure for Biological Research

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funded by the National Science Foundation
Award #ACI-1445604

Key point of this talk

- Inform you about a resource that just happens to be partly here at IU that may be of value to you



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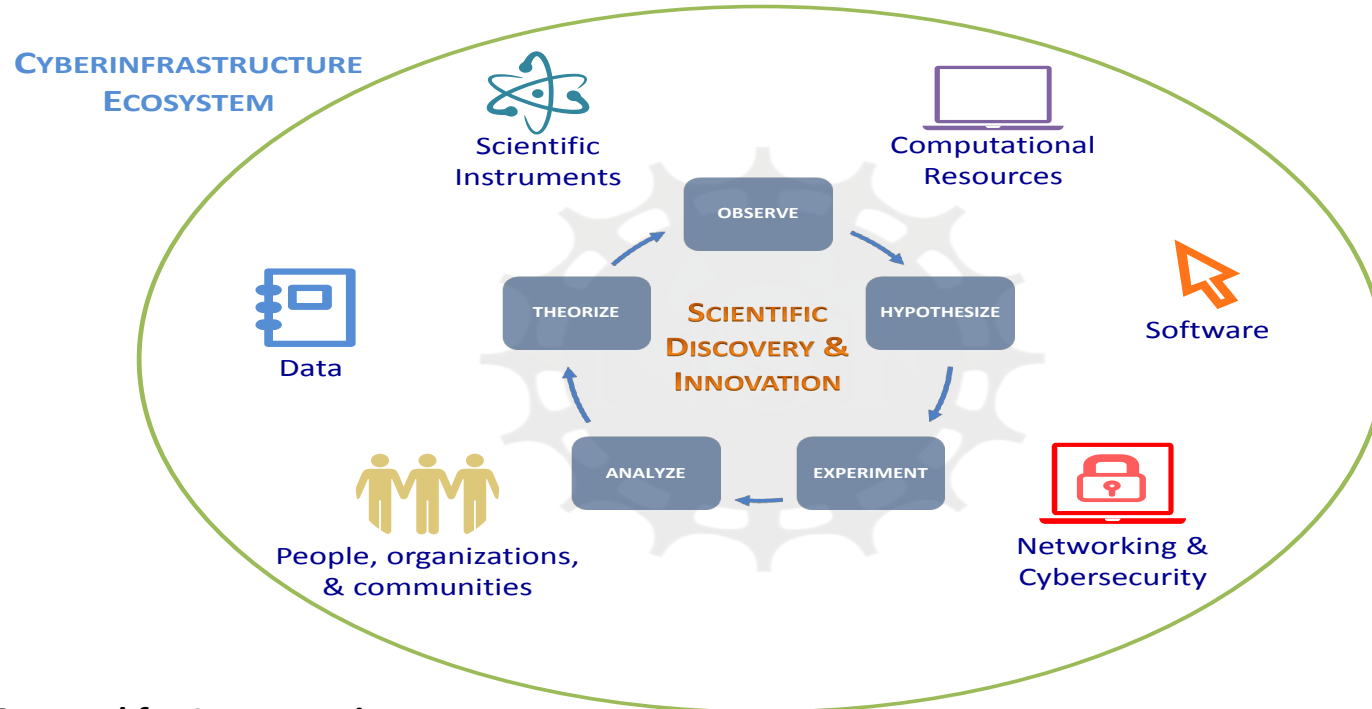


0th slide: language calibration

- Cyberinfrastructure – Cyberinfrastructure consists of computing systems, data storage systems, advanced instruments and data repositories, visualization environments, and people, all linked together by software and high performance networks to improve research productivity and enable breakthroughs not otherwise possible.
- XSEDE – the eXtreme Science and Engineering Discovery Environment – the umbrella support group organization for the major NSF-funded national cyberinfrastructure
- High performance computing (HPC) – large scale computers – big clusters, supercomputers. Typically run in batch mode.
- Cloud computing – on-demand computing, usually using computer resources “someplace else”



NSF embraces an expansive view of cyberinfrastructure motivated by research priorities and the scientific process



Our goal for Jetstream is to serve researchers in the complement of the existing XD program user Community (often working “in the long tail of science”)

Slide source: US National Science Foundation

What is Jetstream?

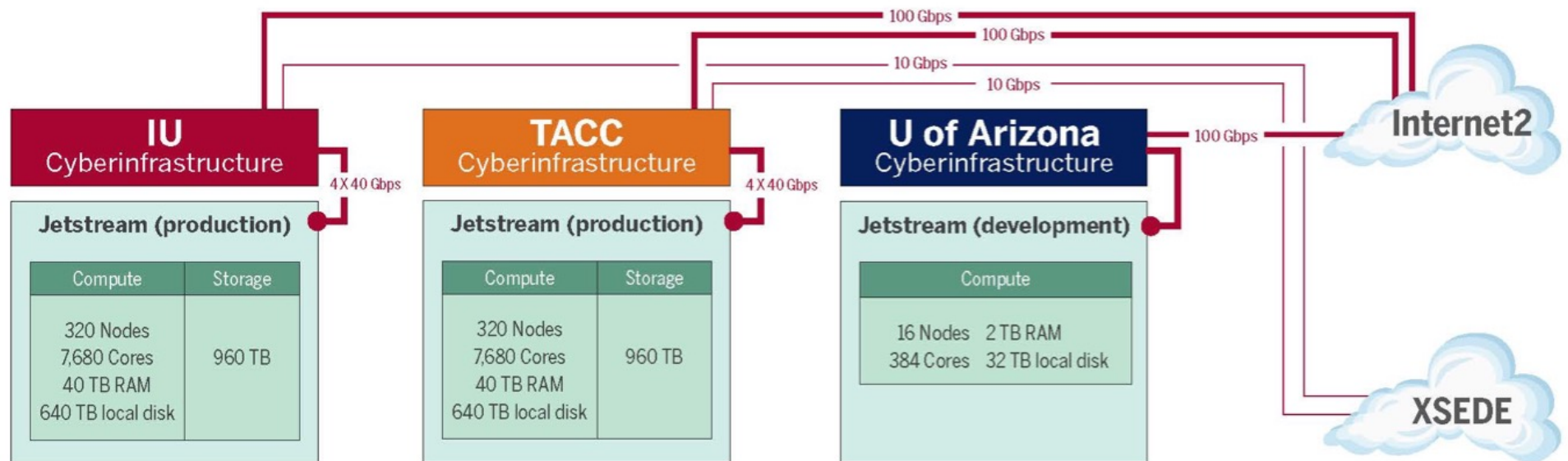
- NSF's first production cloud facility
- Part of the NSF eXtreme Digital (XD) program
- Provides on-demand *interactive* computing and analysis
- Enables *configurable* environments and *programmable cyberinfrastructure*
- User-friendly, widely accessible cloud environment
- User-selectable library of preconfigured virtual machines



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Jetstream

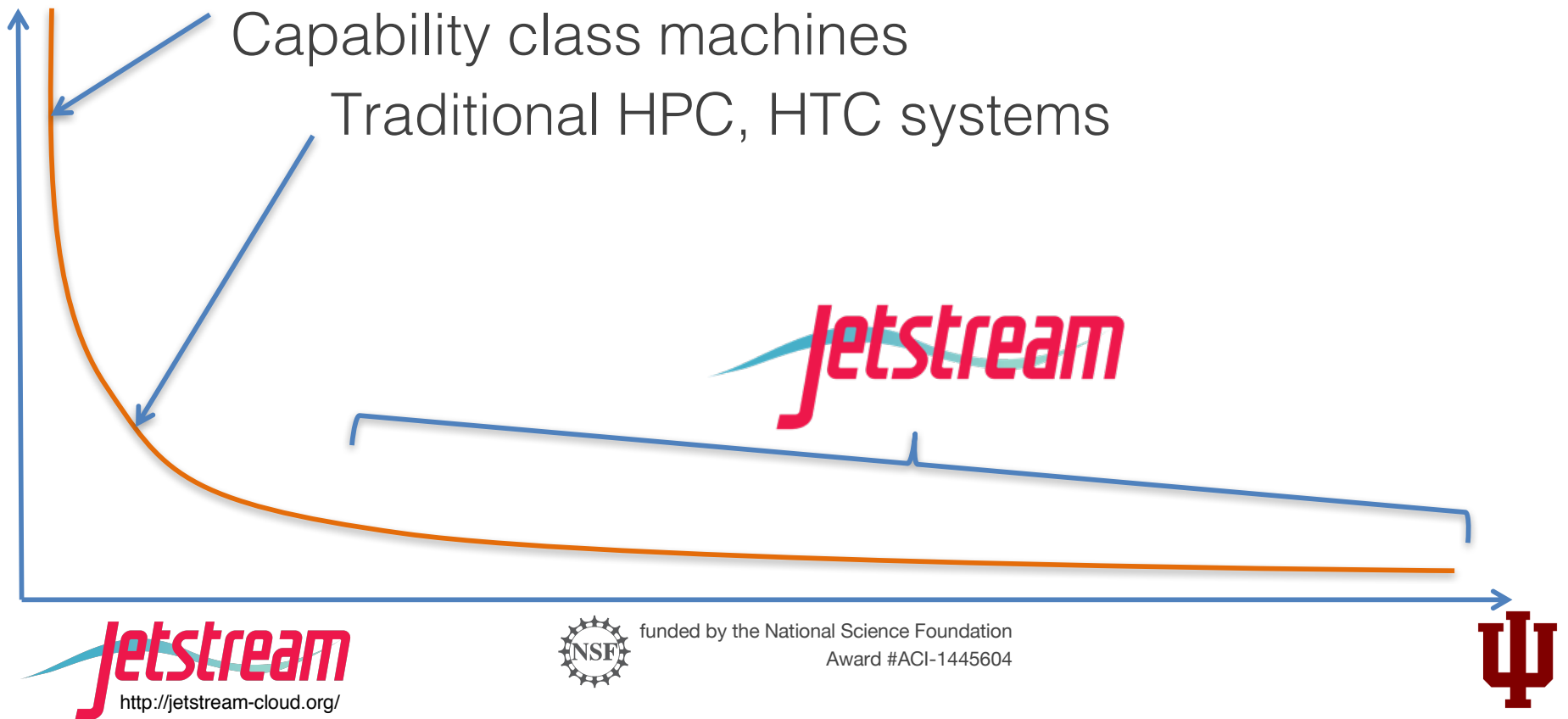


Jetstream provides...

- **"Self-serve" academic cloud services**, enabling researchers or students to select a VM image from a published library, or alternatively to create or customize their own virtual environment for discipline- or task-specific personalized research computing. Authentication to this "self-serve" environment is via Globus using XSEDE credentials.
- **Hosting for persistent Science Gateways**. Jetstream supports persistent science gateways, including the capability of hosting persistent science gateways within a VM when the nature of the gateway is consistent with operation within a VM. Galaxy is one of the initial science gateways supported.
- **Data movement, storage and dissemination.**
 - Jetstream supports data transfer with Globus Connect.
 - Users are able to store VMs in the Indiana University persistent digital repository, IUScholarWorks (scholarworks.iu.edu) and obtain a Digital Object Identifier (DOI) that is associated with the VM stored.
- **Virtual Linux desktop services** delivered from Jetstream to tablet devices. This service is aimed to increase access to Jetstream for users at institutions with limited resources including small schools, schools in EPSCoR states, and Minority Serving Institutions.



Supporting research in the long tail of science



What's special about Jetstream as opposed to other potential approaches to a cloud for NSF

- Atmosphere-based Jetstream Portal
 - Usability-focus
 - Control your own environment (root, network access)
 - Share your VMs as you see fit
- Leveraged support: Involvement of leaders and representatives of VOs, communities of practice, and disciplinary groups
- Dissemination strategy rooted in current best understandings of technology adoption
- Focus on needs as expressed by people who are NOT users of existing XSEDE resources



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Brief Jetstream Almost Live Demo



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Jetstream's Atmosphere Interface

 <https://use.jetstream-cloud.org/> Login

Images Help





SEARCH TAGS

Image Search

Search across image name, tag or description

Showing 86 of 86 images

Featured Images

 BioLinux 8 Mar 22nd 17 04:37 by jfischer	Based on Ubuntu 14.04.3 -Trusty Tahr - server - cloudimg -- **REQUIRES m1.small instance ... bioinformatics desktop Featured gui m1_small Ubuntu x2go
 Ubuntu 14.04.3 Development GUI Mar 22nd 17 04:35 by jfischer	Based on Ubuntu 14.04.3 Development Base Ubuntu 14.04.3 + Xfce + Xfce-goodies, firefox, i ... desktop development Featured gui iRODS Ubuntu vnc
 R with Intel compilers (CentOS ... Mar 22nd 17 04:04 by jfischer	R with Intel compilers built on CentOS 7 (7.3) ** Requires m1.small or greater sized VM * ... CentOS desktop development Featured gui Intel m1_small vnc
 MATLAB (Based on CentOS 6)	MATLAB (Based on CentOS 6)

©2017 Jetstream-Cloud [Feedback & Support](#)



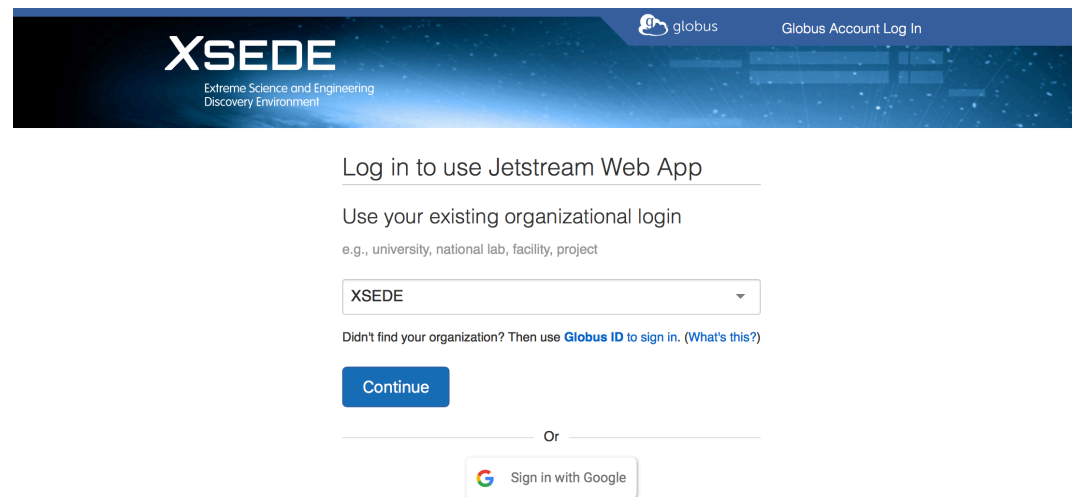
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Jetstream's Atmosphere Interface

Globus Auth under the hood

Pick identity provider

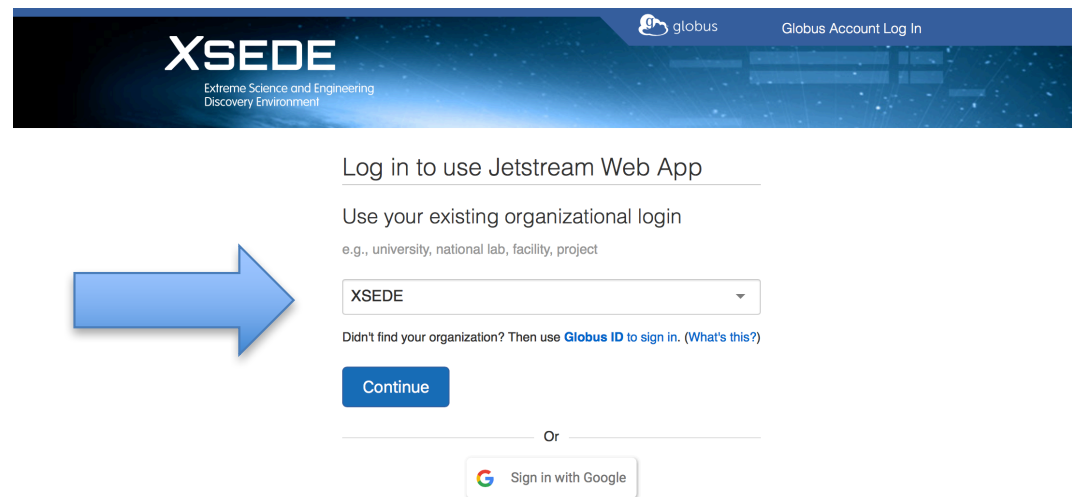


The screenshot shows the XSEDE login page. At the top, there is a header with the XSEDE logo and the text "Extreme Science and Engineering Discovery Environment". To the right of the header, there is a "globus" logo and a "Globus Account Log In" link. Below the header, the main content area has the heading "Log in to use Jetstream Web App". Underneath, it says "Use your existing organizational login" followed by "e.g., university, national lab, facility, project". There is a dropdown menu with "XSEDE" selected. Below the dropdown, it says "Didn't find your organization? Then use [Globus ID to sign in](#). ([What's this?](#))". There is a blue "Continue" button. Below the button, there is a horizontal line with the word "Or" in the center. Below the line, there is a button with the Google logo and the text "Sign in with Google".

Jetstream's Atmosphere Interface

Globus Auth under the hood

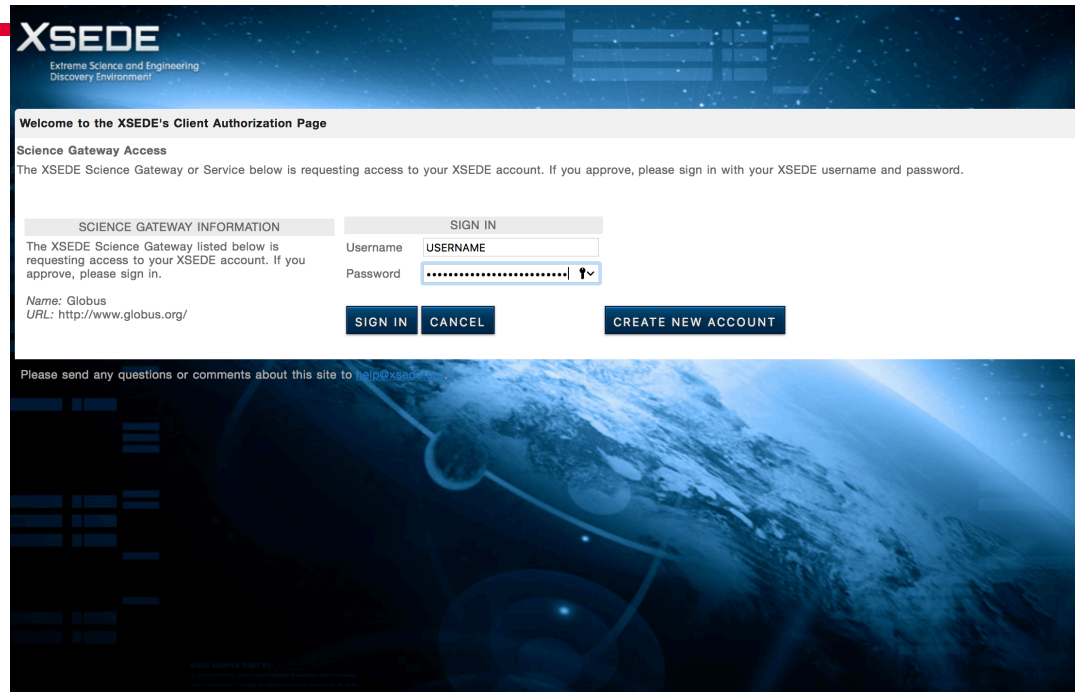
Pick identity provider



The screenshot shows the XSEDE login page. At the top, there's a header with the XSEDE logo and the text 'Extreme Science and Engineering Discovery Environment'. To the right of the header, there's a 'globus' logo and a 'Globus Account Log In' link. Below the header, the main content area has the heading 'Log in to use Jetstream Web App'. Underneath, it says 'Use your existing organizational login' followed by 'e.g., university, national lab, facility, project'. There is a dropdown menu with 'XSEDE' selected. Below the dropdown, it says 'Didn't find your organization? Then use [Globus ID to sign in](#). ([What's this?](#))'. There is a blue 'Continue' button. Below the button, there's an 'Or' separator. At the bottom, there is a 'Sign in with Google' button with the Google logo.

Jetstream's Atmosphere Interface

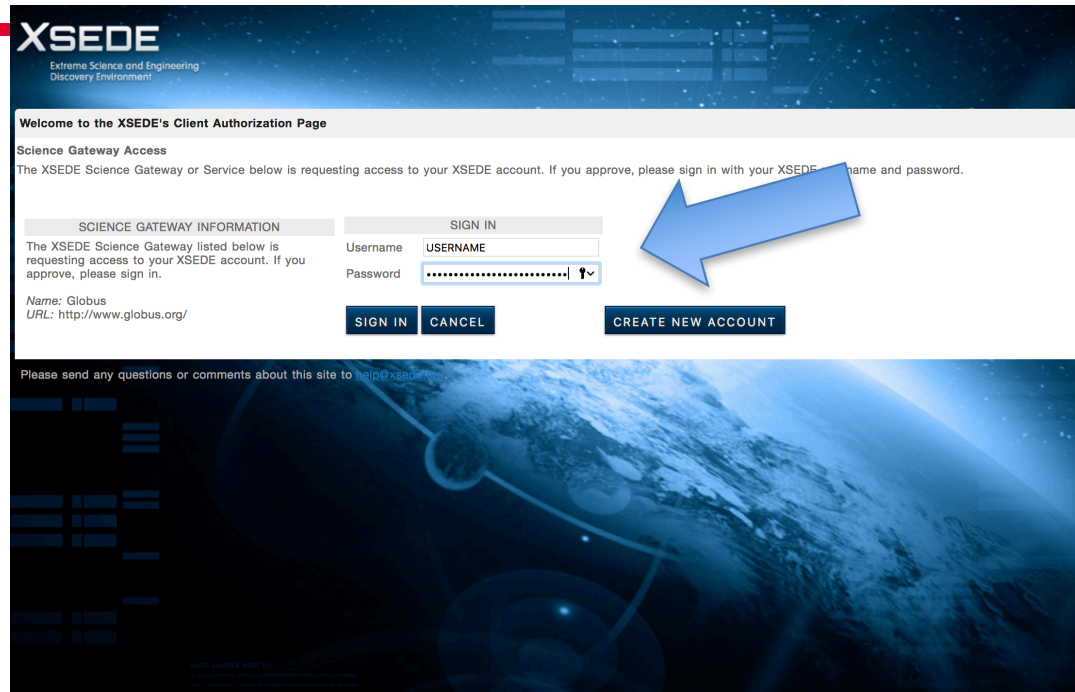
Authenticate with the
chosen identity provider



The screenshot shows the XSEDE Client Authorization Page. At the top, the XSEDE logo is displayed with the tagline "Extreme Science and Engineering Discovery Environment". Below the logo, a heading reads "Welcome to the XSEDE's Client Authorization Page". A section titled "Science Gateway Access" contains a paragraph: "The XSEDE Science Gateway or Service below is requesting access to your XSEDE account. If you approve, please sign in with your XSEDE username and password." Below this text, there are two columns. The left column, titled "SCIENCE GATEWAY INFORMATION", contains the text: "The XSEDE Science Gateway listed below is requesting access to your XSEDE account. If you approve, please sign in." and "Name: Globus URL: http://www.globus.org/". The right column, titled "SIGN IN", contains a "Username" field with the text "USERNAME" and a "Password" field with a masked password "*****" and a dropdown arrow. Below the "SIGN IN" section, there are three buttons: "SIGN IN", "CANCEL", and "CREATE NEW ACCOUNT". At the bottom of the page, there is a footer with the text: "Please send any questions or comments about this site to help@xse.edu".

Jetstream's Atmosphere Interface

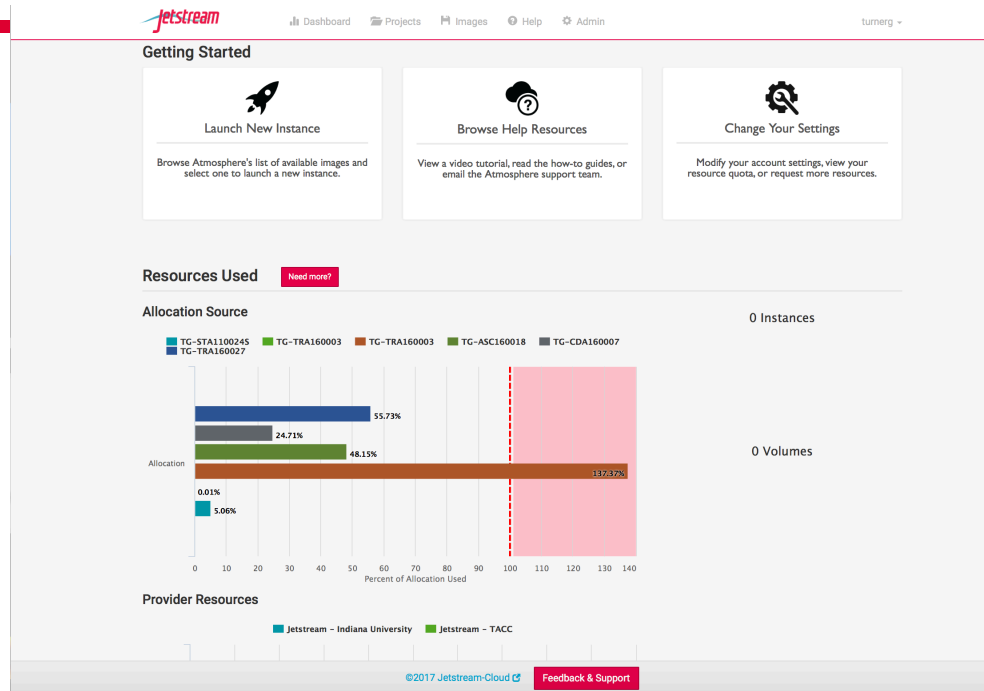
Authenticate with the
chosen identity provider



The screenshot shows the XSEDE Client Authorization Page. At the top, the XSEDE logo is displayed with the tagline "Extreme Science and Engineering Discovery Environment". Below the logo, a welcome message reads: "Welcome to the XSEDE's Client Authorization Page". The main section is titled "Science Gateway Access" and contains the text: "The XSEDE Science Gateway or Service below is requesting access to your XSEDE account. If you approve, please sign in with your XSEDE username and password." Below this text, there are two columns. The left column is titled "SCIENCE GATEWAY INFORMATION" and contains the text: "The XSEDE Science Gateway listed below is requesting access to your XSEDE account. If you approve, please sign in." Below this text, it says "Name: Globus" and "URL: http://www.globus.org/". The right column is titled "SIGN IN" and contains two input fields: "Username" with the placeholder text "USERNAME" and "Password" with a masked password "*****" and a dropdown arrow. Below the input fields are three buttons: "SIGN IN", "CANCEL", and "CREATE NEW ACCOUNT". A large blue arrow points from the right towards the "SIGN IN" button. At the bottom of the page, there is a link to "Please send any questions or comments about this site to help@xse.edu".

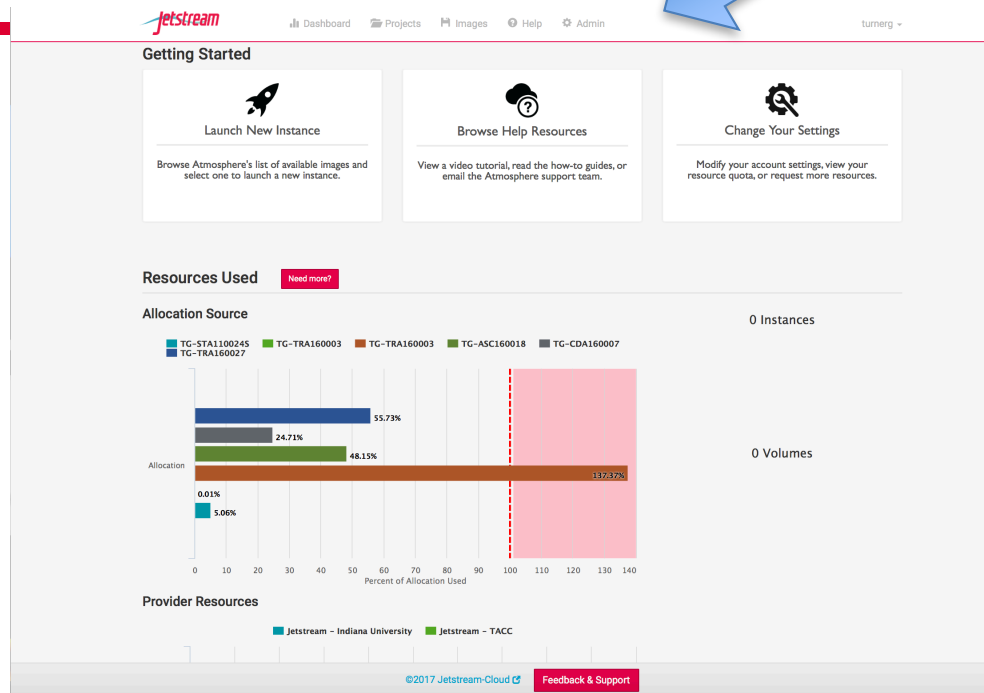
Jetstream's Atmosphere Interface

user's home dashboard



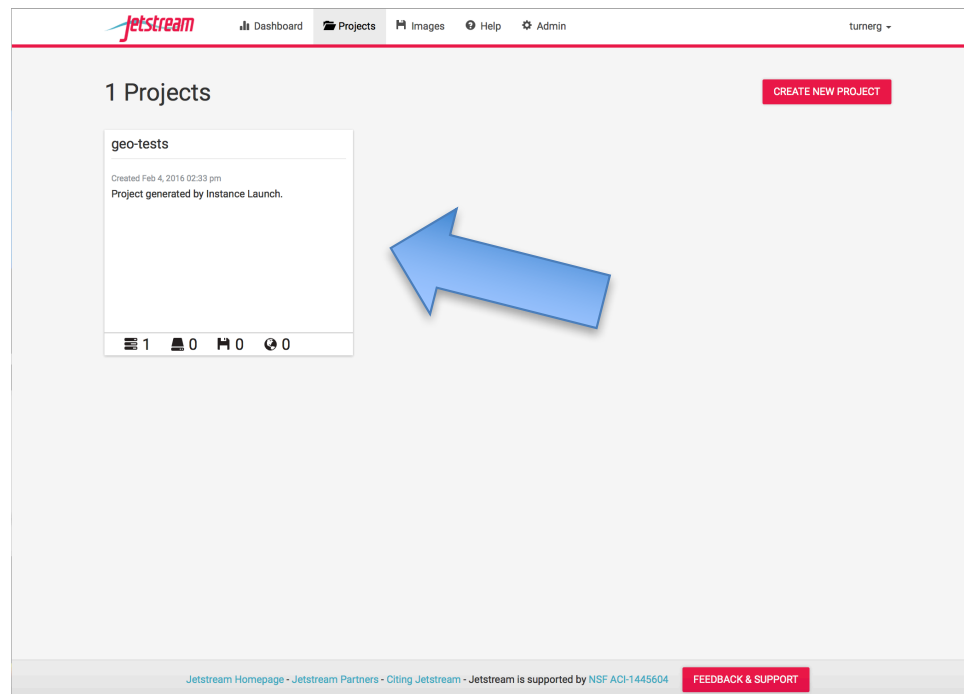
Jetstream's Atmosphere Interface

user's home dashboard



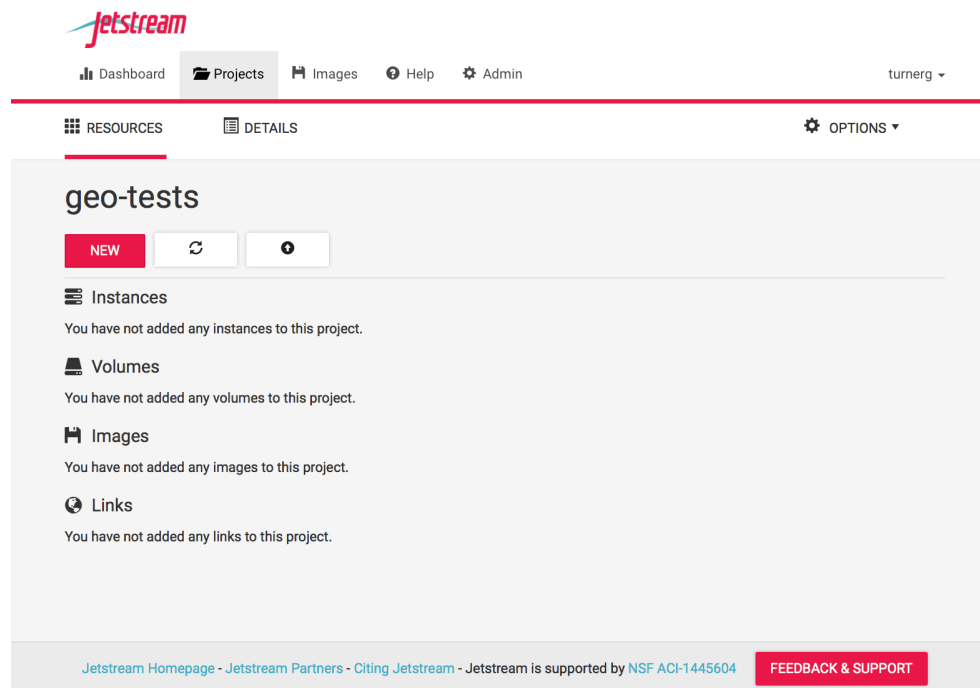
Jetstream's Atmosphere Interface

user's project dashboard



Jetstream's Atmosphere Interface

user's project details



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Jetstream's Atmosphere Interface

Instance ready for use



The screenshot displays the Jetstream Atmosphere web interface. At the top, there is a navigation bar with links for Dashboard, Projects (which is highlighted), Images, Help, and Admin. A user profile 'turnerg' is visible in the top right. Below the navigation bar, there are tabs for RESOURCES and DETAILS, with a gear icon for OPTIONS. The main content area is titled 'geo-tests' and includes buttons for NEW, a refresh icon, and a help icon. Under the 'Instances' section, there is a table with the following data:

Name	Status	Activity	IP Address	Size	Provider
geo-demo-CentOS7-001	Active	N/A	149.165.156.173	M1.Small	Jetstream - Indiana University

Below the table, there are sections for Volumes, Images, and Links, each with a message stating that no items have been added to the project. At the bottom of the interface, there is a footer with links to the Jetstream Homepage, Partners, and Citing Jetstream, along with a note that Jetstream is supported by NSF ACI-1445604 and a FEEDBACK & SUPPORT button.

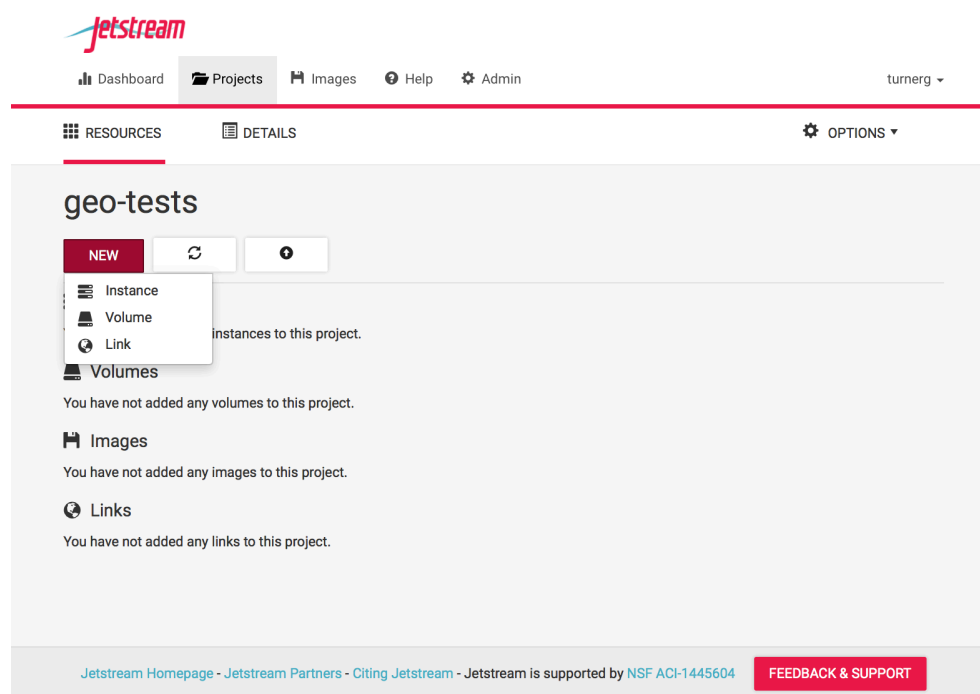


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Jetstream's Atmosphere Interface

starting an instance

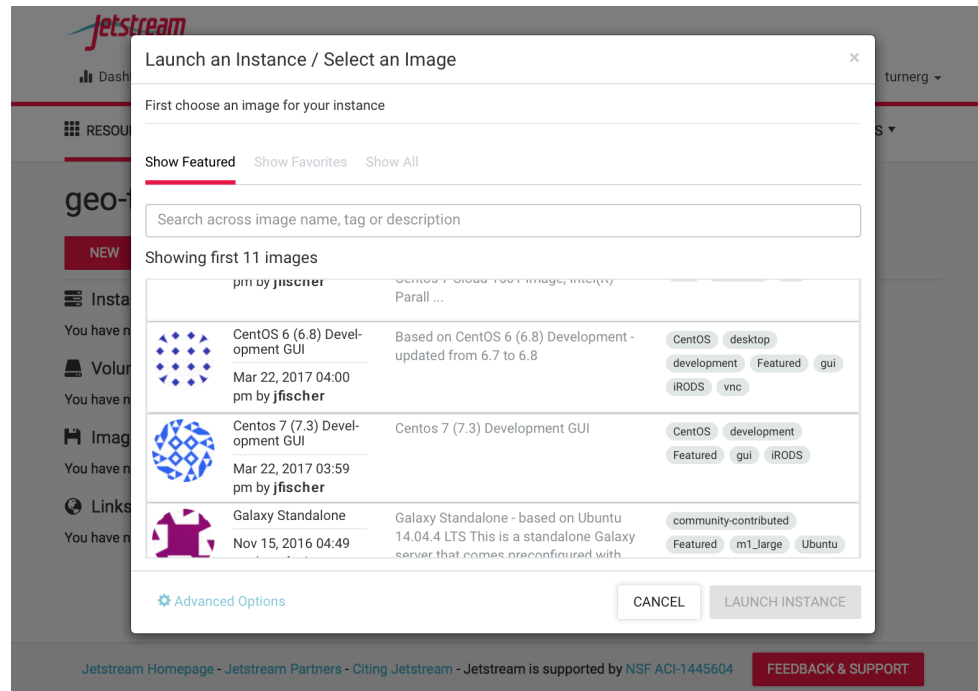


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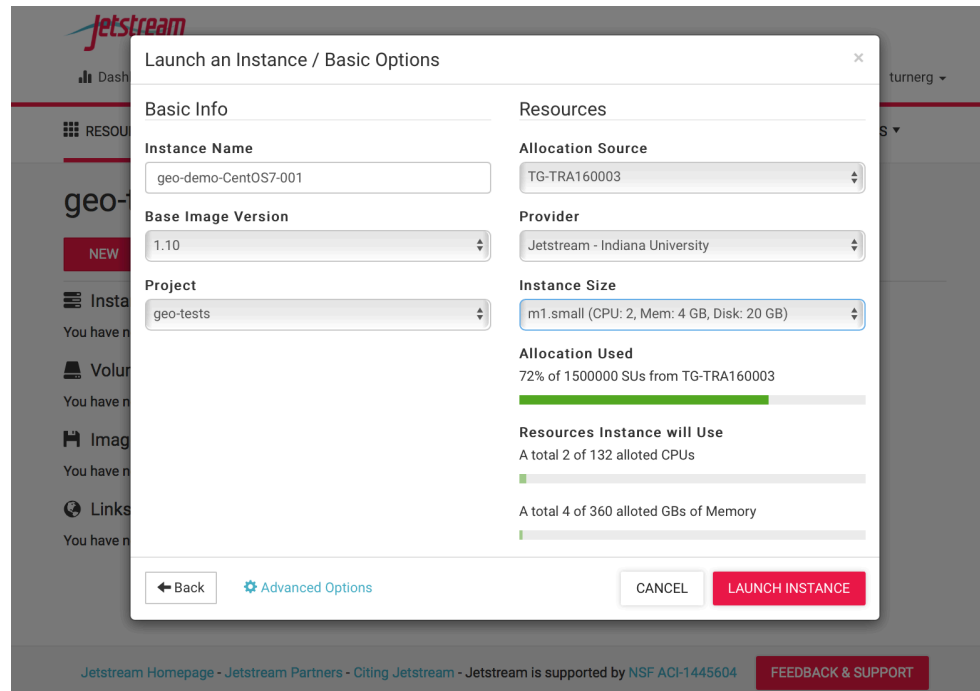
Jetstream's Atmosphere Interface

pick an image from library



Jetstream's Atmosphere Interface

Instance's details; e.g.
name, flavor, allocation, etc.



The screenshot shows the 'Launch an Instance / Basic Options' dialog box in the Jetstream Atmosphere interface. The dialog is divided into two main sections: 'Basic Info' and 'Resources'.

Basic Info:

- Instance Name:** geo-demo-CentOS7-001
- Base Image Version:** 1.10
- Project:** geo-tests

Resources:

- Allocation Source:** TG-TRA160003
- Provider:** Jetstream - Indiana University
- Instance Size:** m1.small (CPU: 2, Mem: 4 GB, Disk: 20 GB)

Allocation Used: 72% of 1500000 SUs from TG-TRA160003

Resources Instance will Use:

- A total 2 of 132 allotted CPUs
- A total 4 of 360 allotted GBs of Memory

At the bottom of the dialog, there are buttons for 'Back', 'Advanced Options', 'CANCEL', and 'LAUNCH INSTANCE'.

Jetstream's Atmosphere Interface

Instance is building

Jetstream

Dashboard Projects Images Help Admin turnerg

RESOURCES DETAILS OPTIONS

geo-tests

NEW

Instances

Name	Status	Activity	IP Address	Size	Provider
geo-demo-CentOS7-001	Build	N/A	N/A		

Volumes

You have not added any volumes to this project.

Images

You have not added any images to this project.

Links

You have not added any links to this project.

[Jetstream Homepage](#) - [Jetstream Partners](#) - [Citing Jetstream](#) - Jetstream is supported by [NSF ACI-1445604](#) [FEEDBACK & SUPPORT](#)

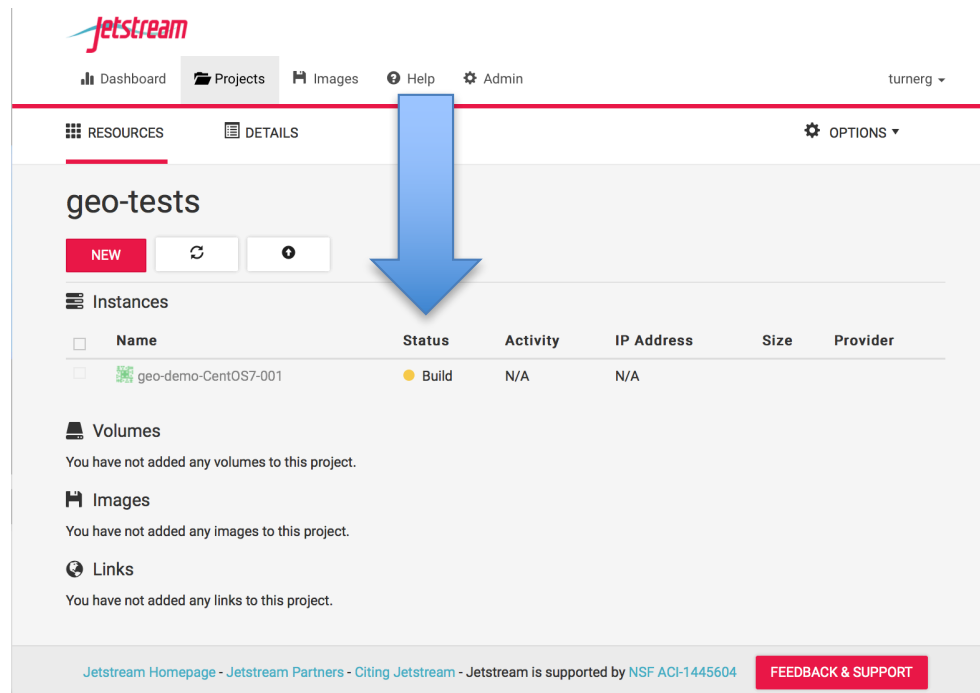


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Jetstream's Atmosphere Interface

Instance is building



The screenshot displays the Jetstream Atmosphere web interface. At the top, there is a navigation bar with links for Dashboard, Projects, Images, Help, and Admin. The user 'turnerg' is logged in. Below the navigation bar, the 'geo-tests' project is selected, showing a 'NEW' button and a refresh icon. A large blue arrow points to the 'Build' status of the instance 'geo-demo-CentOS7-001' in the 'Instances' table. The table has columns for Name, Status, Activity, IP Address, Size, and Provider. Below the table, there are sections for Volumes, Images, and Links, all indicating that no items have been added to this project. At the bottom, there is a footer with links to the Jetstream Homepage, Partners, and Citing Jetstream, along with a 'FEEDBACK & SUPPORT' button.

Name	Status	Activity	IP Address	Size	Provider
geo-demo-CentOS7-001	Build	N/A	N/A		

Jetstream's Atmosphere Interface

...still building

The screenshot shows the Jetstream Atmosphere interface for a project named 'geo-tests'. The interface has a navigation bar with 'Dashboard', 'Projects', 'Images', 'Help', and 'Admin'. The 'Projects' tab is active, showing a list of instances. A blue box highlights the 'Status' and 'Activity' columns of the instance table, and a large blue arrow points to the 'Status' column.

Name	Status	Activity	IP Address	Size	Provider
geo-demo-CentOS7-001	Active	Initializing	172.18.63.4	11.Small	Jetstream - Indiana University

Atmosphere is doing the hard part (systems administration) of virtualized computing



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Jetstream's Atmosphere Interface

...still building

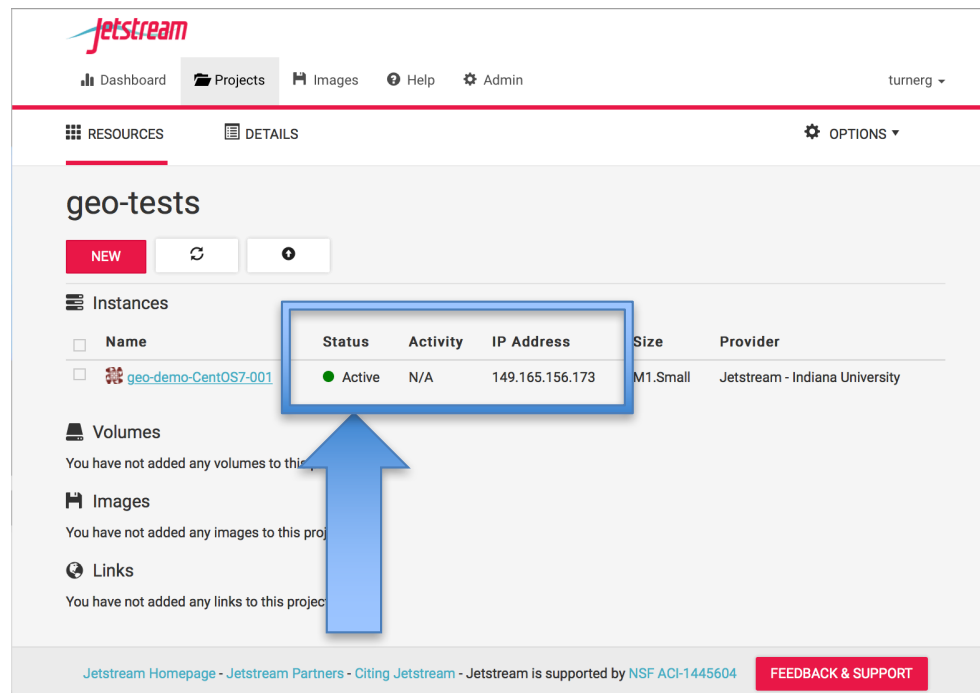
The screenshot shows the Jetstream Atmosphere interface. The top navigation bar includes links for Dashboard, Projects, Images, Help, and Admin. The user 'turnerg' is logged in. The main section is titled 'geo-tests' and contains a 'NEW' button, a refresh icon, and a settings icon. Below this is a table of instances. The table has columns for Name, Status, Activity, IP Address, Size, and Provider. The instance 'geo-demo-CentOS7-001' is highlighted with a blue box, showing a status of 'Active' (yellow dot) and 'Networking' (green bar). A large blue arrow points up to the highlighted row. The footer includes links to the Jetstream Homepage, Partners, and Citing Jetstream, along with a 'FEEDBACK & SUPPORT' button.

Name	Status	Activity	IP Address	Size	Provider
geo-demo-CentOS7-001	Active	Networking	149.165.156.173	M1.Small	Jetstream - Indiana University


Atmosphere is doing the hard part (systems administration) of virtualized computing; e.g. building the network, routers, & virtual switches

Jetstream's Atmosphere Interface

Instance ready for use



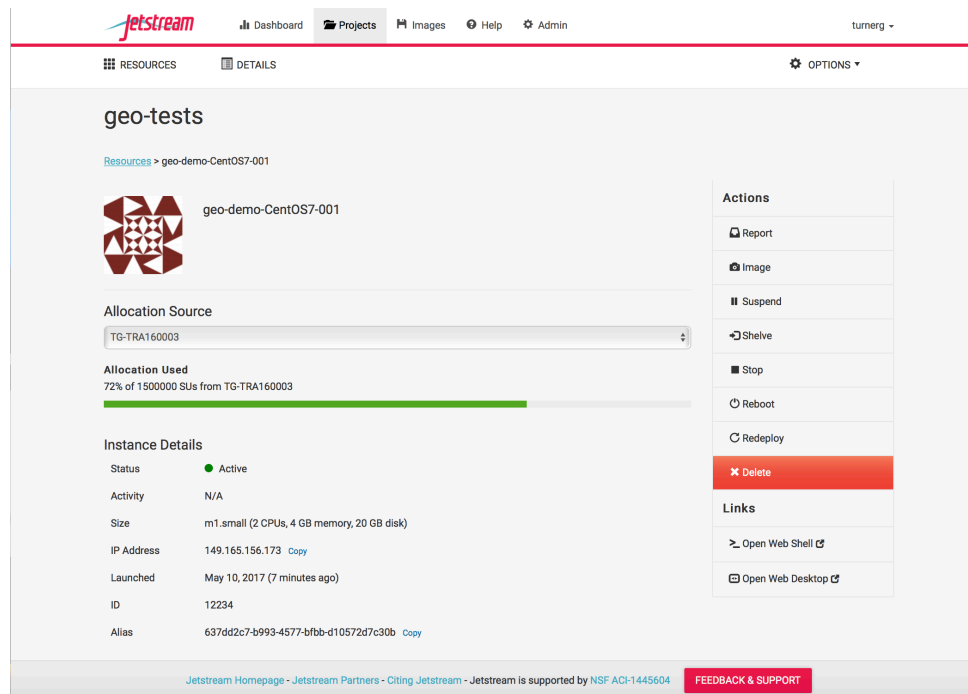
The screenshot shows the Jetstream Atmosphere interface. The top navigation bar includes links for Dashboard, Projects, Images, Help, and Admin. The user 'turnerg' is logged in. The main content area is titled 'geo-tests' and includes a 'NEW' button and a refresh icon. Below this is a section for 'Instances' with a table showing the status of various instances. A blue box highlights the 'Status' column, and a blue arrow points to the 'Active' status of the 'geo-demo-CentOS7-001' instance.

Name	Status	Activity	IP Address	Size	Provider
 geo-demo-CentOS7-001	Active	N/A	149.165.156.173	M1.Small	Jetstream - Indiana University

...and in the end, all you need to do is log in and start doing science & engineering

Jetstream's Atmosphere Interface

User's instance dashboard



The screenshot displays the Jetstream Atmosphere interface for a user named 'turnerg'. The main content area shows the 'geo-tests' instance details. The instance is named 'geo-demo-CentOS7-001' and is currently 'Active'. It is allocated from the source 'TG-TRA160003' and has used 72% of the 1500000 SUs from that source. The instance details table lists the following information:

Instance Details	
Status	Active
Activity	N/A
Size	m1.small (2 CPUs, 4 GB memory, 20 GB disk)
IP Address	149.165.156.173 Copy
Launched	May 10, 2017 (7 minutes ago)
ID	12234
Alias	637dd2c7-b993-4577-bfbb-d10572d7c30b Copy

On the right side, there is an 'Actions' panel with buttons for Report, Image, Suspend, Shelf, Stop, Reboot, Redeploy, and Delete (highlighted in red). Below the actions is a 'Links' panel with buttons for 'Open Web Shell' and 'Open Web Desktop'. The footer of the interface includes links to the Jetstream Homepage, Partners, and Citing Jetstream, along with a note that Jetstream is supported by NSF ACI-1445604 and a 'FEEDBACK & SUPPORT' button.

Jetstream's Atmosphere Interface

User's instance dashboard
Instance's details

Allocation Source
TG-TRA160003

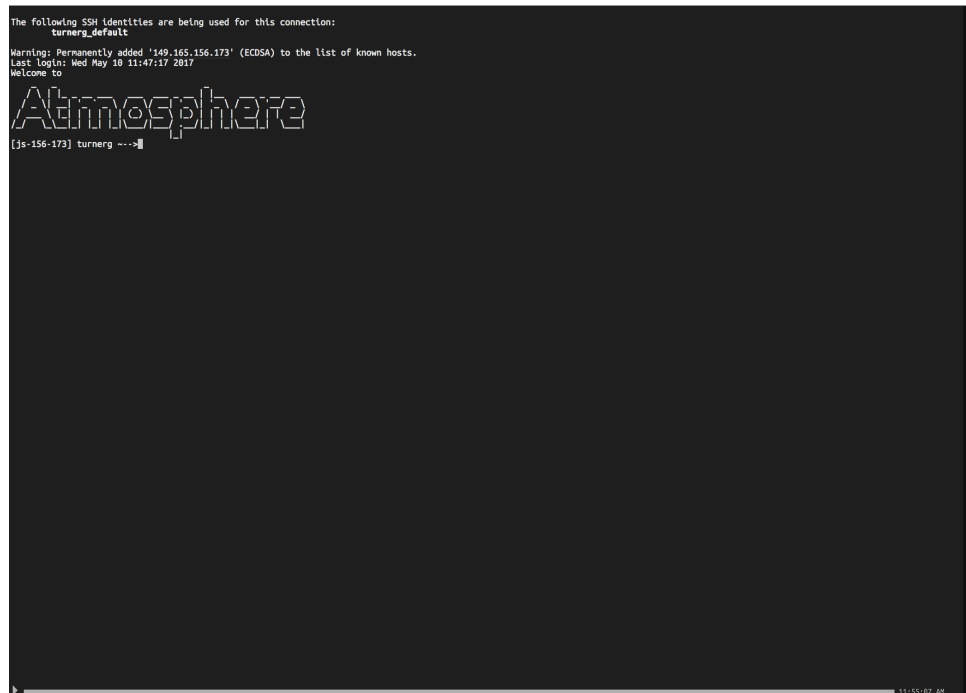
Allocation Used
72% of 1500000 SUs from TG-TRA160003

Instance Details

Status	● Active
Activity	N/A
Size	m1.small (2 CPUs, 4 GB memory, 20 GB disk)
IP Address	149.165.156.173 Copy
Launched	May 10, 2017 (7 minutes ago)
ID	12234
Alias	637dd2c7-b993-4577-bfbb-d10572d7c30b Copy

Jetstream's Atmosphere Interface

Web Shell access to instance
External ssh access also available

A screenshot of a web-based terminal window titled "Atmosphere". The terminal shows a login sequence for the user "turnerg" on a host named "js-156-173". It displays SSH identities, a warning about a new host, and a last login timestamp. The prompt is "[js-156-173] turnerg ---". The interface includes standard window controls (close, maximize, zoom, full screen, star) in the top right corner and a status bar at the bottom right showing "1: Gate One" and the time "11:55:57 AM".

```
The following SSH identities are being used for this connection:
turnerg_default

Warning: Permanently added '149.165.156.173' (ECDSA) to the list of known hosts.
Last login: Wed May 10 11:47:17 2017
Welcome to

Atmosphere
[js-156-173] turnerg ---
```

So what about some biology

- Galaxy
- BioLinux
- CyVerse applications
 - Maker-P
 - From the Brendel Lab
 - Bwasp
 - Bgramose
- Jupyter notebooks
- Whatever you want to run

One exemplar: Douglas Lab and colleagues

Marlis & Michael Douglas



Postdoc



Jeff Pummil – collaborator & campus champion



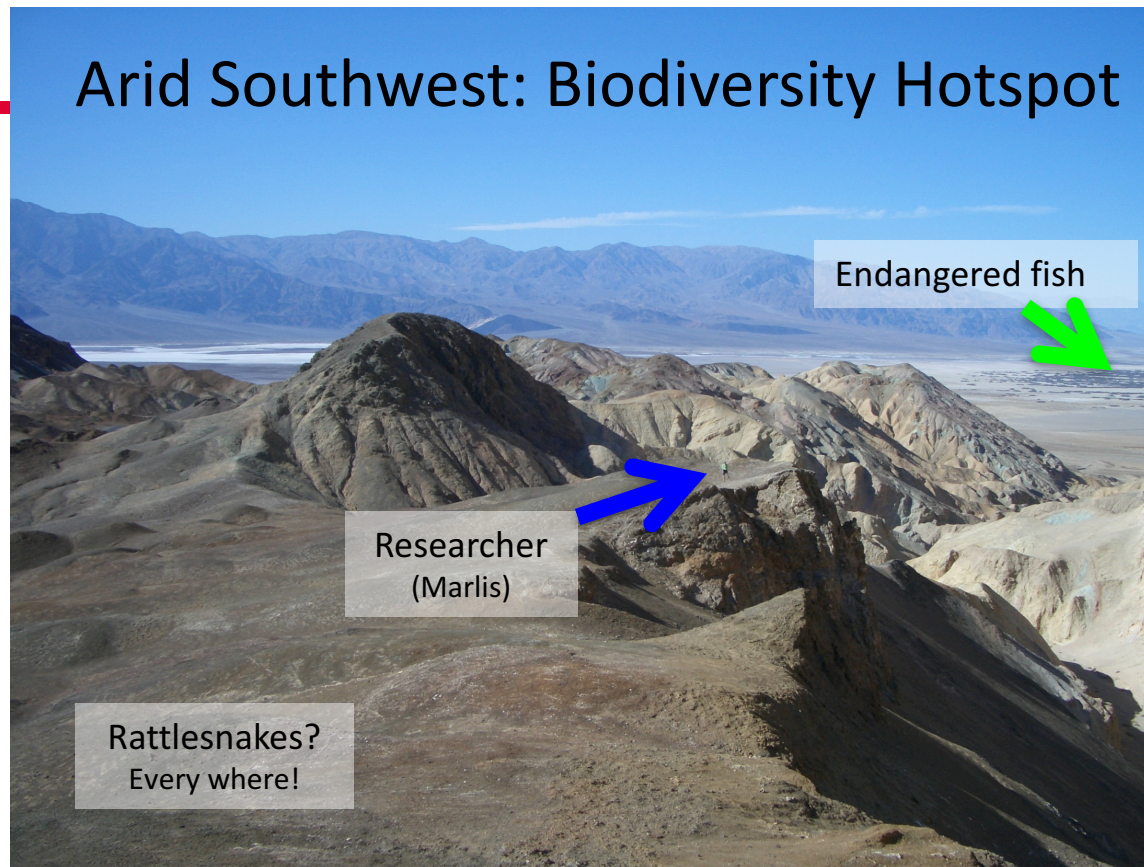
Graduate Students



*Slide courtesy Douglas Lab, University of Arkansas.
Not to be reused without permission from the Douglas Lab*



Arid Southwest: Biodiversity Hotspot



*Slide courtesy Douglas Lab, University of Arkansas.
Not to be reused without permission from the Douglas Lab*



Western Fishes: Conservation

- **Endemic species** with adaptations to desert rivers
- Populations declining due to **habitat alterations** (= dams, stocking of predators, water diversions)
- Most such endemic species are **rare, threatened or endangered**

Ecosystem Change



Endangered



Invasive Species



Study Goals:

- **Clarify biodiversity** within Western Fishes
- Assess geographic patterns in genetic diversity
- Evaluate historic + current hybridization to test for gene flow between species

Slide courtesy Douglas Lab, University of Arkansas. Not to be reused without permission from the Douglas Lab

Data: ddRAD (double-digest Restriction-Associated-DNA)

- Genomic Methods:
 - Extract genomic DNA from snake blood or fish fins
 - Cut genome in small fragments (~ 500 base pair)
 - Subsample ~40-60K fragments to reduce genome size
 - Sequence fragments with Next-Generation-Sequencing
 - 1 Illumina HiSeq lane: generates ~140 million reads
- ddRAD Project:
 - 6-8 HiSeq lanes / project
 - 400-800 samples of fish or snakes



= relatively
large data
sets

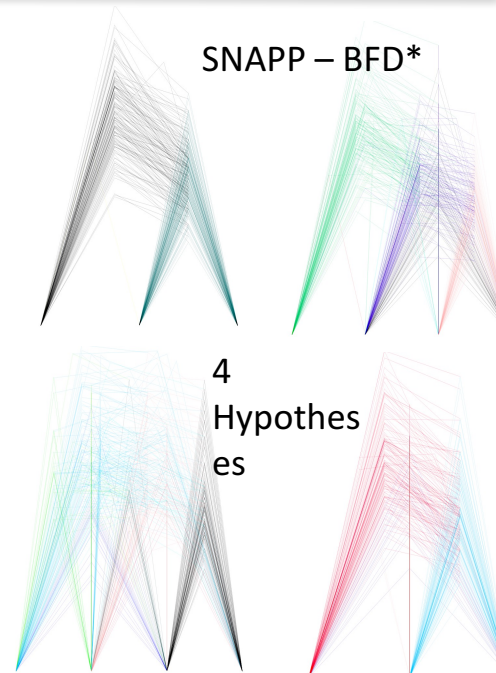
*Slide courtesy Douglas Lab,
University of Arkansas. Not
to be reused without
permission from the
Douglas Lab*



Western Fishes: Analyses on Jetstream

Bayes Factor Delimitation (BFD) (Species delimitation)

- Compares phylogenetic hypotheses
 - Incorporates thousands of loci
 - Integrates over gene tree topologies
- Computationally intensive
 - MCMC algorithm
 - Millions of iterations



Scaling Science and Community expertise for using cloud with Jetstream

Nirav Merchant

nirav@email.arizona.edu

University of Arizona

WQ-MAKER Workflow: Background

MAKER-P is a flexible and scalable genome annotation pipeline that automates the many steps necessary for the detection of protein coding genes (Campbell et al. 2013)

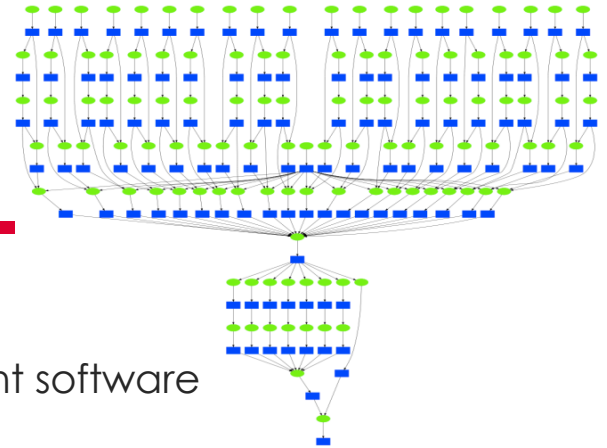
MAKER-P identifies repeats, aligns ESTs and proteins to a genome, produces ab initio gene predictions, and automatically synthesizes these data into gene annotations having evidence-based quality indices

MAKER-P is developed by the Yandell Lab (Univ. of Utah)

MAKER-P needs more resources to support researcher activity than CyVerse itself has readily available



WQ-MAKER Workflow: Background



Limitations of MAKER

- Installation of MAKER is challenging and complex with significant software dependencies (suitable for dedicated/single user HPC systems)
- MAKER runs are not time efficient
- On CyVerse, most users can only run a few instances using Maker-P

CCTOOLS developed by Dough Thain (Notre Dame) includes Makeflow and Work queue task distribution system

Allows scaling from single instance to multiple instances

Includes support for popular bioinformatics tool

Easy to customize and develop new workflows using simple make like syntax



Work-Queue MAKER community of users

Genome	Sequences	Number of runs	Number of workers per run	Run time (in hours)
Sporobolus species A	11,789 contigs	9	22	144
Sporobolus species B	6615 contigs	9	21-35	108
Brassica rapa	44,000 scaffolds	1	10	4
Zea mays W22	10 chromosomes	1	25	1440
Zea mays nc350	6460 scaffolds	1	22	72
Culex tarsalis	7478 scaffolds	3	40	120
MP29 (peach x plum)	5003 scaffolds	3	40	48
Pigweed	4126 scaffolds	1	20	120
Sclerotiana homeocarpa isolate 10	231 contigs	3	10	6
Sclerotiana homeocarpa isolate 11	257 contigs	3	10	6
Calypste anna	265 super scaffolds	1	10	8
Kochia scoparia	19,671 scaffolds	3	21	72

Table showing detailing the use of WQ-MAKER on Jetstream


Number of distinct users	16
Number of genomes annotated	18
Number of runs	50
Number of instances launched	788

Summary table of the genome annotated and number of instances launched from WQ-MAKER




How do you get access to Jetstream?


- Go to xse.de and make an account on the XSEDE portal
- Send a mail note to help@jetstream-cloud.org We'll walk you through the process of a startup allocation
- That takes just a few days
- Then one of the following:
 - After you get some experience with a startup allocation then send email again to help@jetstream-cloud.org and we will help you through the process of applying through a full application proposal
 - OR....if you have a good idea now of what you need, contact us ASAP and we will try to help you get a proposal in by the Oct 15 deadline for the current round


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[Ecosystem](#)
[Community Engagement](#)
[News](#)

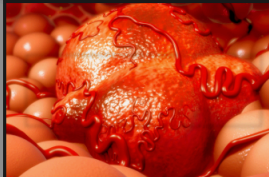
XUP



ROSIE Blooms
Science Gateway shares biomolecular data with the nation's scientists and researchers



Supporting LIGO Gravitational Wave Detections
The Laser Interferometer Gravitational-Wave Observatory (LIGO) has used XSEDE resources since 2013




Identifying Cancer DNA Changes With XSEDE Resources
Many groups, like the University of Pittsburgh Cancer Institute, have turned to XSEDE for help.


XSEDE is a single virtual system that scientists can use to interactively share computing resources, data and expertise. People around the world use these resources and services — things like supercomputers, collections of data and new tools — to improve our planet.

- [Getting Started Guide](#)
- [Science Success Stories](#)
- [Diversity and Inclusion Programs](#)
- [XSEDE's Project Documents](#)

GET STARTED WITH XSEDE




Researchers
The National Science Foundation's eXtreme Digital (XD) program is making new infrastructure and next-generation digital services available to researchers and educators to handle the huge volumes of digital information




Service Providers
Service Providers - entities that make a resource visible and coordinated with the national cyberinfrastructure for benefit to the research community - are central to the function of XSEDE.


NEWS AND EVENTS



CIPRES: One facet in bold NSF vision
The CIPRES science gateway: A NSF investment launching thousands of scientific publications with...
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Dance With Algae
XSEDE resources help researchers create human-like movement
[View »](#)



HPC for all at XSEDE16 Conference
The first five years of the NSF-funded XSEDE project culminated in an exciting and enlightening...
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SUBMISSION PERIOD	ALLOCATION BEGIN DATE
Dec 15 thru Jan 15	April 1
Mar 15 thru Apr 15	Jul 1
Jun 15 thru Jul 15	Oct 1
Sep 15 thru Oct 15	Jan 1

And.... We have people to help you with biological research (ncgas.org)



NCGAS Highlights

Meeting Cenicafe at PAG 2017 to discuss
Coffee Genomics
Trinity and NCGAS Partnership thrives as
software popularity continues to grow
NCGAS provides HPC training and
networking to Bethune Cookman University

NCGAS Home

The mission of the National Center for Genome Analysis Support is to enable the biological research community of the US to analyze, understand, and make use of the vast amount of genomic information now available. NCGAS focuses particularly on transcriptome- and genome-level assembly, phylogenetics, metagenomics/transcriptomics and community genomics.

What we planned and what we learned

Planned:

- Jetstream is a managed science cloud – a cloud managed for science
- Community “self-service” works quite well
- Use in research and research education

Learned:

- Jetstream is “programmable cyberinfrastructure”
- Some of the contexts in which Jetstream has been useful in education



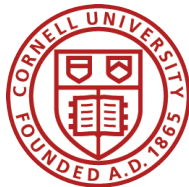
Jetstream partner organizations

Acquisition and Management & Operations partners



Management & Operations partners

Application / community lead partners



funded by the National Science Foundation
Award #ACI-1445604



Questions and discussion?



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